Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2023 – 12:49 PM EST

PDB ID	:	1RUH
Title	:	RHINOVIRUS 14 MUTANT N1219S COMPLEXED WITH ANTIVIRAL COMPOUND WIN 52084
Authors	:	Hadfield, A.; Oliveira, M.A.; Kim, K.H.; Minor, I.; Kremer, M.J.; Heinz, B.A.; Shepard, D.; Pevear, D.C.; Rueckert, R.R.; Rossmann, M.G.
Deposited on	:	1995-06-09
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

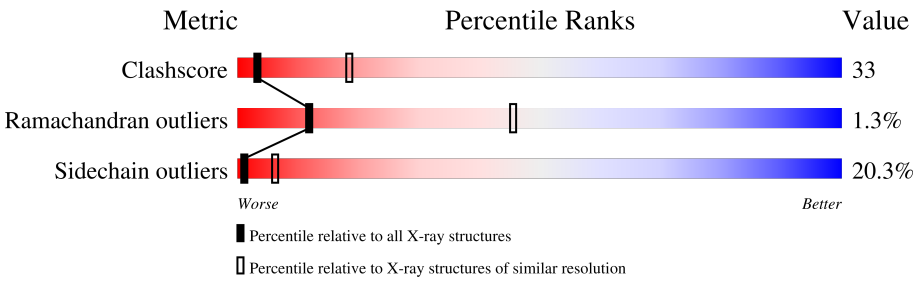
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	289	33% 39% 16% 6% 6%
2	2	262	43% 36% 13% 5% •
3	3	236	42% 36% 17% 6%
4	4	68	18% 16% 16% 9% 41%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6292 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RHINOVIRUS 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	273	2168	1372	374	414	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	219	SER	ASN	engineered mutation	UNP P03303

- Molecule 2 is a protein called RHINOVIRUS 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	255	1952	1238	330	372	12	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	170	LEU	ILE	conflict	UNP P03303

- Molecule 3 is a protein called RHINOVIRUS 14.

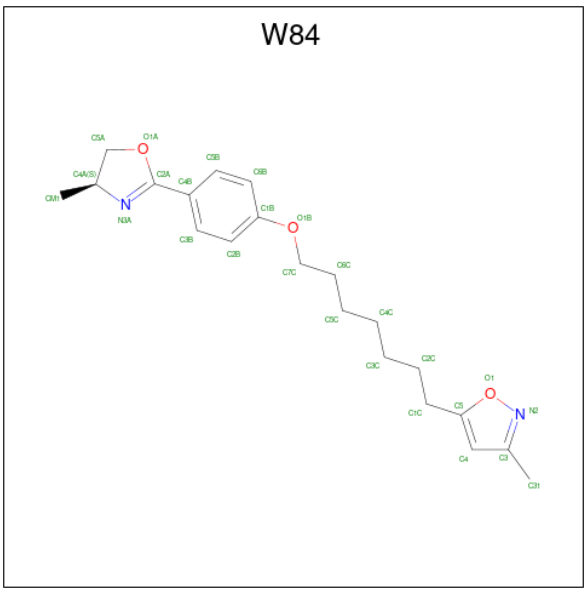
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	236	1849	1184	305	353	7	0	0	0

- Molecule 4 is a protein called RHINOVIRUS 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	4	40	297	186	47	62	2	0	0	0

- Molecule 5 is 5-(7-(5-HYDRO-4-METHYL-2-OXAZOLYL)PHENOXY)HEPTYL)-3-MET

HYL ISOXAZOLE (three-letter code: W84) (formula: $C_{21}H_{28}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	1	1	26	21	2	3	0	0

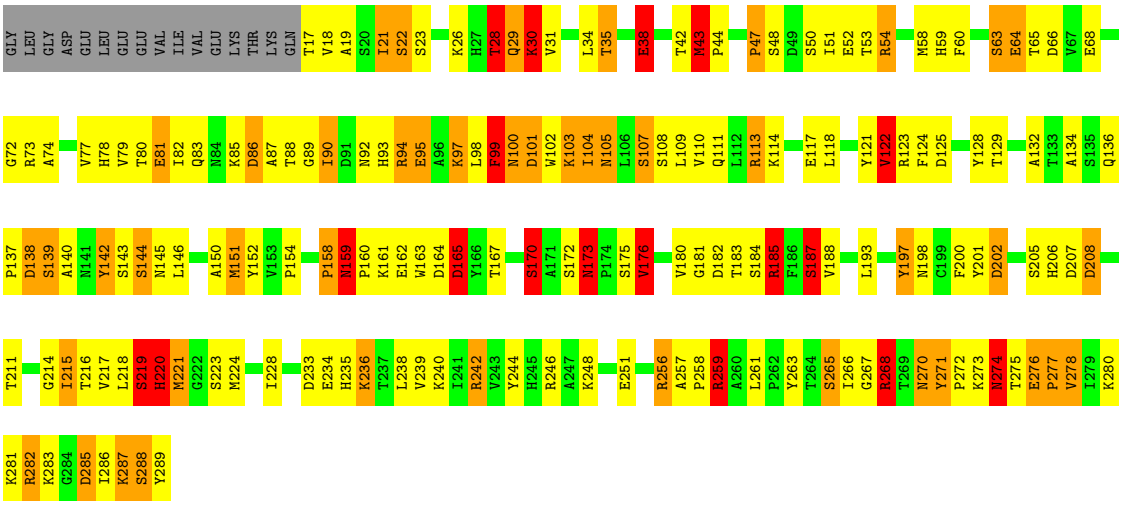
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

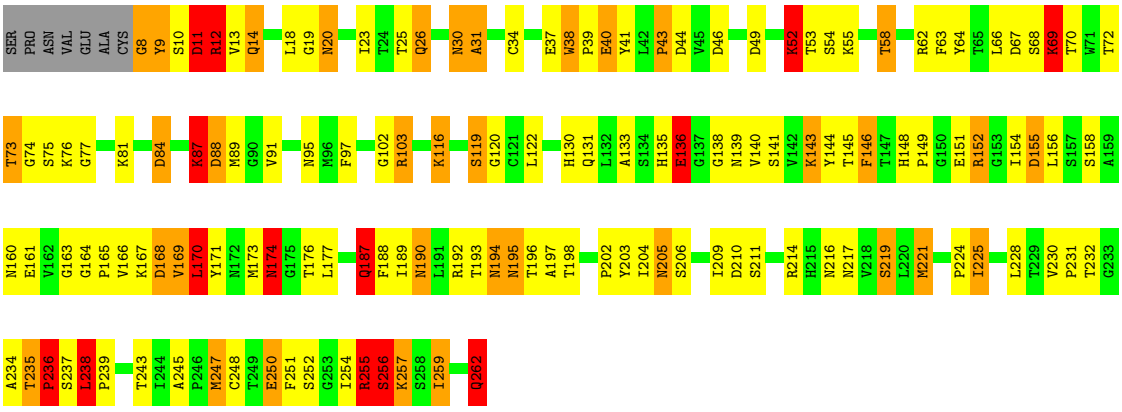
• Molecule 1: RHINOVIRUS 14

Chain 1: 33% 39% 16% 6% 6%



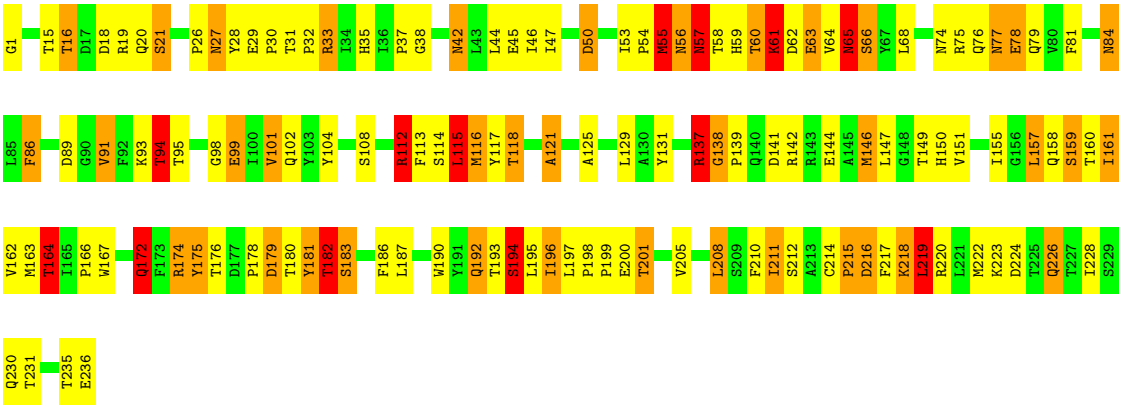
• Molecule 2: RHINOVIRUS 14

Chain 2: 43% 36% 13% 5%



• Molecule 3: RHINOVIRUS 14

Chain 3: 42% 36% 17% 6%



- Molecule 4: RHINOVIRUS 14

Chain 4:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	445.10Å 445.10Å 445.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6292	wwPDB-VP
Average B, all atoms ($Å^2$)	1.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: W84

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	1.95	40/2226 (1.8%)	2.35	120/3028 (4.0%)
2	2	1.85	32/2001 (1.6%)	2.17	79/2735 (2.9%)
3	3	1.76	21/1898 (1.1%)	2.16	75/2597 (2.9%)
4	4	2.30	13/302 (4.3%)	2.46	21/406 (5.2%)
All	All	1.88	106/6427 (1.6%)	2.24	295/8766 (3.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	4
2	2	0	2
All	All	0	6

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	220	HIS	C-N	-25.12	0.76	1.34
1	1	219	SER	C-N	-18.77	0.90	1.34
1	1	170	SER	CB-OG	-14.30	1.23	1.42
1	1	150	ALA	C-N	14.03	1.66	1.34
1	1	285	ASP	CA-CB	11.82	1.79	1.53
4	4	42	GLY	N-CA	11.71	1.63	1.46
4	4	40	SER	CB-OG	10.77	1.56	1.42
2	2	256	SER	CB-OG	10.25	1.55	1.42
1	1	95	GLU	CB-CG	10.12	1.71	1.52
4	4	44	SER	CB-OG	9.95	1.55	1.42
4	4	41	ALA	C-O	9.40	1.41	1.23
1	1	117	GLU	CD-OE1	9.38	1.35	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	175	SER	CB-OG	-9.13	1.30	1.42
1	1	38	GLU	CB-CG	-9.05	1.34	1.52
1	1	187	SER	CB-OG	-8.87	1.30	1.42
1	1	63	SER	CB-OG	-8.75	1.30	1.42
3	3	21	SER	CA-CB	8.74	1.66	1.52
2	2	248	CYS	CB-SG	-8.67	1.67	1.82
3	3	57	ASN	CA-CB	8.43	1.75	1.53
2	2	40	GLU	CD-OE1	8.22	1.34	1.25
1	1	288	SER	CA-CB	8.04	1.65	1.52
2	2	52	LYS	CE-NZ	7.92	1.68	1.49
3	3	1	GLY	N-CA	7.83	1.57	1.46
3	3	63	GLU	CD-OE1	7.73	1.34	1.25
2	2	219	SER	CA-CB	-7.70	1.41	1.52
1	1	283	LYS	N-CA	7.66	1.61	1.46
2	2	136	GLU	CB-CG	7.55	1.66	1.52
1	1	234	GLU	CD-OE1	7.42	1.33	1.25
4	4	33	LYS	CE-NZ	7.42	1.67	1.49
1	1	282	ARG	CD-NE	7.37	1.58	1.46
3	3	108	SER	CB-OG	7.37	1.51	1.42
2	2	152	ARG	CD-NE	7.23	1.58	1.46
1	1	187	SER	N-CA	7.16	1.60	1.46
2	2	152	ARG	CZ-NH2	7.03	1.42	1.33
2	2	194	ASN	CA-CB	6.97	1.71	1.53
4	4	46	SER	CB-OG	6.93	1.51	1.42
3	3	164	THR	C-O	6.92	1.36	1.23
4	4	51	LYS	CE-NZ	6.78	1.66	1.49
3	3	61	LYS	CE-NZ	6.71	1.65	1.49
2	2	256	SER	C-O	6.68	1.36	1.23
1	1	72	GLY	C-O	6.52	1.34	1.23
1	1	30	LYS	CE-NZ	6.50	1.65	1.49
1	1	81	GLU	CD-OE1	6.42	1.32	1.25
2	2	8	GLY	N-CA	6.42	1.55	1.46
2	2	12	ARG	NE-CZ	6.41	1.41	1.33
1	1	283	LYS	CE-NZ	6.37	1.65	1.49
1	1	52	GLU	C-O	6.33	1.35	1.23
3	3	138	GLY	N-CA	6.33	1.55	1.46
2	2	87	LYS	CB-CG	-6.29	1.35	1.52
1	1	30	LYS	CD-CE	6.26	1.67	1.51
3	3	194	SER	CB-OG	-6.26	1.34	1.42
4	4	33	LYS	CD-CE	6.08	1.66	1.51
3	3	50	ASP	CA-CB	-6.08	1.40	1.53
1	1	94	ARG	CD-NE	6.00	1.56	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	108	SER	CA-CB	-5.99	1.44	1.52
3	3	99	GLU	CB-CG	-5.96	1.40	1.52
4	4	54	GLU	CD-OE1	5.94	1.32	1.25
2	2	102	GLY	N-CA	5.89	1.54	1.46
1	1	285	ASP	N-CA	-5.85	1.34	1.46
2	2	11	ASP	CA-CB	5.69	1.66	1.53
1	1	158	PRO	CA-C	-5.67	1.41	1.52
1	1	175	SER	CA-CB	-5.65	1.44	1.52
4	4	37	SER	CB-OG	-5.64	1.34	1.42
2	2	168	ASP	C-O	5.63	1.34	1.23
3	3	45	GLU	CD-OE1	5.63	1.31	1.25
3	3	172	GLN	CG-CD	-5.63	1.38	1.51
2	2	235	THR	C-N	-5.62	1.23	1.34
4	4	63	GLY	N-CA	5.62	1.54	1.46
1	1	97	LYS	CD-CE	5.61	1.65	1.51
2	2	187	GLN	N-CA	5.58	1.57	1.46
4	4	45	LEU	C-N	5.56	1.46	1.34
3	3	222	MET	CG-SD	5.54	1.95	1.81
2	2	219	SER	CB-OG	-5.45	1.35	1.42
1	1	73	ARG	C-O	5.43	1.33	1.23
2	2	236	PRO	C-O	5.43	1.34	1.23
1	1	276	GLU	CD-OE1	5.42	1.31	1.25
4	4	50	SER	CB-OG	5.40	1.49	1.42
2	2	262	GLN	CD-OE1	5.39	1.35	1.24
2	2	187	GLN	CB-CG	-5.39	1.38	1.52
2	2	54	SER	CA-CB	-5.38	1.44	1.52
1	1	267	GLY	C-O	5.35	1.32	1.23
1	1	94	ARG	NE-CZ	5.33	1.40	1.33
2	2	40	GLU	CB-CG	5.30	1.62	1.52
3	3	118	THR	CB-OG1	5.28	1.53	1.43
1	1	117	GLU	CD-OE2	-5.27	1.19	1.25
2	2	68	SER	CB-OG	-5.26	1.35	1.42
1	1	246	ARG	CZ-NH2	5.25	1.39	1.33
1	1	175	SER	N-CA	5.25	1.56	1.46
1	1	251	GLU	CA-CB	-5.24	1.42	1.53
3	3	33	ARG	CZ-NH2	5.22	1.39	1.33
2	2	74	GLY	C-O	5.21	1.31	1.23
2	2	120	GLY	N-CA	5.19	1.53	1.46
2	2	161	GLU	CA-CB	-5.16	1.42	1.53
1	1	283	LYS	CD-CE	5.11	1.64	1.51
2	2	136	GLU	CD-OE1	5.11	1.31	1.25
1	1	68	GLU	CD-OE2	-5.10	1.20	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	38	GLY	CA-C	-5.10	1.43	1.51
2	2	12	ARG	CZ-NH2	5.10	1.39	1.33
1	1	26	LYS	CB-CG	-5.09	1.38	1.52
2	2	38	TRP	CG-CD1	5.08	1.43	1.36
3	3	77	ASN	C-O	5.08	1.33	1.23
1	1	202	ASP	CA-CB	-5.08	1.42	1.53
2	2	58	THR	C-O	5.06	1.32	1.23
3	3	86	PHE	CA-CB	-5.04	1.42	1.53
3	3	30	PRO	N-CD	-5.04	1.40	1.47
1	1	288	SER	C-O	5.03	1.32	1.23

All (295) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	246	ARG	NE-CZ-NH1	22.50	131.55	120.30
1	1	256	ARG	NE-CZ-NH2	20.44	130.52	120.30
1	1	123	ARG	NE-CZ-NH1	19.20	129.90	120.30
2	2	255	ARG	NE-CZ-NH2	-18.68	110.96	120.30
1	1	285	ASP	CB-CG-OD1	-17.64	102.43	118.30
2	2	87	LYS	CA-CB-CG	17.64	152.21	113.40
1	1	256	ARG	NE-CZ-NH1	-16.96	111.82	120.30
3	3	137	ARG	NE-CZ-NH1	-16.90	111.85	120.30
1	1	94	ARG	NE-CZ-NH2	-16.50	112.05	120.30
3	3	216	ASP	CB-CG-OD2	16.15	132.84	118.30
1	1	282	ARG	NE-CZ-NH2	-14.11	113.24	120.30
2	2	255	ARG	NE-CZ-NH1	13.94	127.27	120.30
1	1	165	ASP	CB-CG-OD2	13.04	130.04	118.30
1	1	197	TYR	N-CA-CB	-12.92	87.34	110.60
2	2	168	ASP	CB-CG-OD1	-12.82	106.76	118.30
1	1	185	ARG	NE-CZ-NH1	12.32	126.46	120.30
3	3	50	ASP	CA-CB-CG	12.23	140.30	113.40
1	1	94	ARG	CD-NE-CZ	-12.04	106.75	123.60
2	2	11	ASP	CB-CG-OD1	-11.72	107.75	118.30
2	2	194	ASN	N-CA-CB	-11.54	89.83	110.60
2	2	193	THR	C-N-CA	11.39	150.19	121.70
1	1	170	SER	CA-CB-OG	11.11	141.20	111.20
3	3	215	PRO	C-N-CA	11.00	149.20	121.70
2	2	152	ARG	NE-CZ-NH2	-10.99	114.81	120.30
4	4	41	ALA	CA-C-N	10.88	137.96	116.20
4	4	48	ASP	CB-CG-OD1	-10.86	108.53	118.30
3	3	19	ARG	NE-CZ-NH2	10.71	125.66	120.30
3	3	33	ARG	NE-CZ-NH2	-10.63	114.98	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	285	ASP	CB-CG-OD2	10.62	127.85	118.30
1	1	197	TYR	CA-CB-CG	10.60	133.55	113.40
1	1	285	ASP	CA-CB-CG	-10.46	90.39	113.40
3	3	50	ASP	CB-CG-OD1	10.46	127.71	118.30
2	2	151	GLU	CA-CB-CG	10.40	136.28	113.40
1	1	246	ARG	NE-CZ-NH2	-10.13	115.23	120.30
1	1	187	SER	CB-CA-C	10.07	129.24	110.10
1	1	282	ARG	CD-NE-CZ	-10.04	109.55	123.60
1	1	246	ARG	CD-NE-CZ	10.01	137.61	123.60
1	1	159	ASN	CB-CA-C	9.88	130.16	110.40
3	3	57	ASN	N-CA-CB	-9.83	92.90	110.60
1	1	208	ASP	CB-CG-OD1	-9.81	109.47	118.30
3	3	146	MET	CG-SD-CE	9.80	115.89	100.20
3	3	216	ASP	CB-CG-OD1	-9.75	109.52	118.30
1	1	113	ARG	NE-CZ-NH2	-9.73	115.44	120.30
2	2	88	ASP	CB-CG-OD1	-9.69	109.58	118.30
1	1	242	ARG	NE-CZ-NH2	-9.45	115.58	120.30
1	1	54	ARG	CD-NE-CZ	-9.38	110.47	123.60
1	1	66	ASP	CB-CG-OD2	-9.19	110.03	118.30
3	3	57	ASN	CB-CA-C	-9.06	92.28	110.40
2	2	11	ASP	CA-CB-CG	-8.98	93.64	113.40
1	1	38	GLU	CA-CB-CG	8.89	132.95	113.40
3	3	112	ARG	NE-CZ-NH2	-8.81	115.89	120.30
3	3	137	ARG	NE-CZ-NH2	8.80	124.70	120.30
3	3	182	THR	CA-CB-CG2	8.57	124.40	112.40
1	1	165	ASP	CB-CG-OD1	-8.53	110.62	118.30
1	1	285	ASP	N-CA-CB	-8.51	95.28	110.60
1	1	268	ARG	CD-NE-CZ	-8.45	111.77	123.60
1	1	175	SER	CB-CA-C	8.41	126.07	110.10
1	1	123	ARG	CD-NE-CZ	8.38	135.33	123.60
1	1	63	SER	CB-CA-C	-8.37	94.20	110.10
1	1	165	ASP	CB-CA-C	-8.34	93.71	110.40
2	2	250	GLU	CA-CB-CG	8.33	131.72	113.40
1	1	285	ASP	CB-CA-C	-8.32	93.75	110.40
3	3	172	GLN	CB-CG-CD	8.25	133.05	111.60
1	1	187	SER	N-CA-CB	-8.20	98.20	110.50
1	1	251	GLU	CA-CB-CG	8.19	131.42	113.40
2	2	152	ARG	NE-CZ-NH1	8.19	124.39	120.30
4	4	45	LEU	N-CA-CB	-8.13	94.13	110.40
3	3	224	ASP	CB-CG-OD1	-8.11	111.00	118.30
2	2	255	ARG	CA-CB-CG	8.04	131.08	113.40
2	2	11	ASP	OD1-CG-OD2	8.03	138.55	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	4	48	ASP	OD1-CG-OD2	8.02	138.54	123.30
1	1	38	GLU	CB-CG-CD	8.00	135.79	114.20
3	3	181	TYR	CB-CG-CD2	-7.99	116.21	121.00
1	1	95	GLU	OE1-CD-OE2	7.98	132.88	123.30
2	2	219	SER	CA-CB-OG	7.84	132.37	111.20
4	4	47	MET	CA-CB-CG	-7.84	99.98	113.30
1	1	121	TYR	CB-CG-CD1	-7.70	116.38	121.00
2	2	155	ASP	CB-CG-OD1	-7.70	111.37	118.30
3	3	21	SER	CB-CA-C	-7.69	95.50	110.10
2	2	187	GLN	CA-CB-CG	7.61	130.14	113.40
3	3	78	GLU	OE1-CD-OE2	7.58	132.40	123.30
1	1	219	SER	CA-C-N	-7.55	100.60	117.20
2	2	11	ASP	C-N-CA	7.54	140.54	121.70
1	1	173	ASN	N-CA-CB	-7.53	97.04	110.60
1	1	277	PRO	N-CD-CG	-7.53	91.91	103.20
1	1	123	ARG	NE-CZ-NH2	-7.51	116.54	120.30
2	2	170	LEU	CA-CB-CG	7.51	132.57	115.30
1	1	182	ASP	CB-CG-OD1	-7.48	111.57	118.30
2	2	187	GLN	CB-CA-C	7.46	125.33	110.40
3	3	112	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	1	259	ARG	CA-CB-CG	-7.36	97.22	113.40
2	2	214	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	1	282	ARG	NH1-CZ-NH2	7.27	127.40	119.40
1	1	117	GLU	CG-CD-OE2	7.25	132.81	118.30
3	3	142	ARG	CA-CB-CG	7.20	129.24	113.40
2	2	194	ASN	CA-CB-CG	-7.15	97.67	113.40
2	2	190	ASN	CA-CB-CG	7.08	128.98	113.40
1	1	197	TYR	CB-CA-C	7.06	124.52	110.40
3	3	137	ARG	CD-NE-CZ	-7.04	113.74	123.60
3	3	121	ALA	CB-CA-C	-7.03	99.55	110.10
3	3	28	TYR	CB-CG-CD1	-7.02	116.79	121.00
2	2	168	ASP	N-CA-CB	-7.02	97.97	110.60
1	1	185	ARG	NH1-CZ-NH2	-7.01	111.69	119.40
2	2	256	SER	CA-C-O	-7.00	105.39	120.10
1	1	68	GLU	CG-CD-OE2	6.99	132.29	118.30
4	4	41	ALA	CA-C-O	-6.97	105.46	120.10
1	1	42	THR	CA-CB-CG2	6.91	122.08	112.40
1	1	28	THR	CB-CA-C	-6.90	92.96	111.60
1	1	26	LYS	CA-CB-CG	6.87	128.51	113.40
1	1	113	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	1	125	ASP	CB-CG-OD1	-6.87	112.11	118.30
3	3	194	SER	N-CA-CB	-6.77	100.34	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	4	37	SER	CB-CA-C	6.77	122.96	110.10
2	2	136	GLU	CG-CD-OE1	-6.76	104.78	118.30
3	3	163	MET	CA-CB-CG	-6.73	101.86	113.30
2	2	146	PHE	CB-CG-CD1	-6.67	116.13	120.80
2	2	103	ARG	CD-NE-CZ	-6.66	114.28	123.60
3	3	216	ASP	N-CA-CB	-6.65	98.63	110.60
1	1	265	SER	N-CA-CB	-6.63	100.55	110.50
3	3	45	GLU	CG-CD-OE2	6.62	131.54	118.30
3	3	57	ASN	CA-CB-CG	-6.62	98.84	113.40
3	3	27	ASN	CB-CA-C	-6.59	97.22	110.40
2	2	87	LYS	CB-CG-CD	6.58	128.70	111.60
1	1	276	GLU	OE1-CD-OE2	6.56	131.17	123.30
1	1	94	ARG	NH1-CZ-NH2	6.56	126.61	119.40
1	1	68	GLU	CG-CD-OE1	-6.55	105.20	118.30
1	1	288	SER	CB-CA-C	-6.54	97.68	110.10
1	1	53	THR	CA-CB-OG1	-6.53	95.30	109.00
2	2	203	TYR	CB-CG-CD2	6.49	124.89	121.00
3	3	174	ARG	NE-CZ-NH2	6.49	123.55	120.30
4	4	45	LEU	CB-CA-C	6.49	122.53	110.20
3	3	74	ASN	CA-CB-CG	-6.48	99.15	113.40
1	1	288	SER	N-CA-CB	-6.46	100.80	110.50
1	1	22	SER	N-CA-CB	-6.46	100.81	110.50
3	3	183	SER	N-CA-CB	-6.45	100.82	110.50
1	1	274	ASN	O-C-N	6.44	133.01	122.70
1	1	176	VAL	CB-CA-C	-6.43	99.18	111.40
3	3	55	MET	CA-CB-CG	-6.42	102.39	113.30
2	2	168	ASP	OD1-CG-OD2	6.41	135.49	123.30
3	3	29	GLU	CB-CG-CD	6.41	131.52	114.20
2	2	97	PHE	CB-CG-CD1	-6.41	116.32	120.80
1	1	150	ALA	O-C-N	6.39	132.93	122.70
1	1	271	TYR	CB-CG-CD1	6.31	124.79	121.00
3	3	65	ASN	CA-CB-CG	-6.31	99.52	113.40
3	3	16	THR	N-CA-CB	-6.29	98.35	110.30
1	1	95	GLU	CB-CG-CD	-6.28	97.25	114.20
4	4	44	SER	CA-C-N	-6.26	103.43	117.20
2	2	38	TRP	N-CA-CB	-6.25	99.34	110.60
3	3	27	ASN	CA-CB-CG	-6.25	99.66	113.40
3	3	63	GLU	CG-CD-OE1	-6.24	105.83	118.30
3	3	19	ARG	CA-CB-CG	6.23	127.10	113.40
1	1	122	VAL	N-CA-CB	-6.18	97.90	111.50
1	1	219	SER	C-N-CA	-6.16	106.30	121.70
2	2	69	LYS	CA-CB-CG	6.16	126.94	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	136	GLU	CB-CG-CD	-6.15	97.58	114.20
2	2	203	TYR	CB-CG-CD1	-6.14	117.32	121.00
1	1	117	GLU	CG-CD-OE1	-6.11	106.09	118.30
1	1	97	LYS	CD-CE-NZ	-6.10	97.67	111.70
3	3	222	MET	CG-SD-CE	-6.10	90.45	100.20
3	3	219	LEU	CA-CB-CG	6.08	129.28	115.30
2	2	235	THR	CA-CB-CG2	-6.07	103.90	112.40
2	2	219	SER	CB-CA-C	6.07	121.62	110.10
1	1	86	ASP	CB-CG-OD1	6.06	123.75	118.30
3	3	66	SER	CB-CA-C	6.06	121.61	110.10
1	1	164	ASP	C-N-CA	6.05	136.82	121.70
2	2	119	SER	N-CA-CB	6.05	119.57	110.50
1	1	118	LEU	CA-CB-CG	6.04	129.19	115.30
3	3	179	ASP	CB-CG-OD2	6.04	123.73	118.30
1	1	221	MET	CG-SD-CE	6.03	109.85	100.20
2	2	67	ASP	CA-CB-CG	-6.02	100.15	113.40
1	1	224	MET	CG-SD-CE	6.01	109.82	100.20
2	2	103	ARG	CA-CB-CG	6.00	126.61	113.40
2	2	247	MET	CB-CA-C	5.99	122.39	110.40
4	4	48	ASP	CB-CG-OD2	-5.99	112.91	118.30
4	4	61	LEU	CB-CG-CD2	-5.98	100.84	111.00
3	3	1	GLY	N-CA-C	5.96	128.01	113.10
3	3	58	THR	CA-CB-CG2	-5.94	104.08	112.40
1	1	268	ARG	NE-CZ-NH2	-5.93	117.34	120.30
2	2	12	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	1	257	ALA	N-CA-CB	-5.91	101.83	110.10
3	3	45	GLU	CG-CD-OE1	-5.90	106.50	118.30
1	1	35	THR	N-CA-CB	-5.90	99.09	110.30
1	1	256	ARG	CD-NE-CZ	-5.88	115.37	123.60
1	1	94	ARG	CG-CD-NE	-5.88	99.46	111.80
2	2	256	SER	CA-C-N	5.86	130.09	117.20
1	1	236	LYS	CD-CE-NZ	-5.85	98.25	111.70
4	4	30	ASN	CA-CB-CG	-5.84	100.55	113.40
2	2	31	ALA	N-CA-CB	5.84	118.27	110.10
2	2	214	ARG	NE-CZ-NH2	-5.83	117.38	120.30
2	2	238	LEU	N-CA-CB	-5.83	98.74	110.40
3	3	27	ASN	O-C-N	5.80	131.98	122.70
4	4	33	LYS	CD-CE-NZ	-5.79	98.38	111.70
1	1	151	MET	CG-SD-CE	5.78	109.45	100.20
1	1	28	THR	OG1-CB-CG2	5.76	123.25	110.00
2	2	255	ARG	CB-CG-CD	5.76	126.58	111.60
2	2	68	SER	N-CA-CB	-5.75	101.88	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	77	ASN	CA-C-N	5.75	129.85	117.20
1	1	233	ASP	CB-CG-OD2	-5.74	113.13	118.30
2	2	73	THR	CA-CB-OG1	-5.74	96.94	109.00
3	3	147	LEU	CA-CB-CG	5.74	128.49	115.30
1	1	274	ASN	N-CA-CB	5.73	120.92	110.60
1	1	95	GLU	CA-CB-CG	-5.72	100.82	113.40
2	2	52	LYS	CD-CE-NZ	-5.70	98.59	111.70
3	3	1	GLY	O-C-N	-5.70	113.58	122.70
1	1	48	SER	CA-C-O	-5.69	108.14	120.10
1	1	246	ARG	NH1-CZ-NH2	-5.68	113.15	119.40
2	2	161	GLU	CA-CB-CG	5.68	125.90	113.40
2	2	75	SER	N-CA-CB	-5.66	102.02	110.50
4	4	44	SER	O-C-N	5.62	131.69	122.70
3	3	164	THR	N-CA-CB	-5.61	99.65	110.30
3	3	94	THR	O-C-N	5.56	131.60	122.70
2	2	210	ASP	N-CA-CB	-5.55	100.61	110.60
3	3	175	TYR	CB-CA-C	-5.54	99.33	110.40
2	2	84	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	1	122	VAL	CB-CA-C	5.53	121.90	111.40
1	1	202	ASP	CA-CB-CG	5.51	125.52	113.40
4	4	44	SER	C-N-CA	-5.50	107.96	121.70
2	2	12	ARG	CD-NE-CZ	-5.49	115.92	123.60
3	3	112	ARG	CA-CB-CG	5.49	125.47	113.40
2	2	9	TYR	CB-CA-C	5.48	121.37	110.40
1	1	81	GLU	CG-CD-OE1	-5.48	107.34	118.30
1	1	26	LYS	CD-CE-NZ	-5.46	99.13	111.70
3	3	186	PHE	CB-CG-CD1	-5.46	116.98	120.80
2	2	43	PRO	N-CD-CG	-5.46	95.01	103.20
1	1	43	MET	CG-SD-CE	5.45	108.93	100.20
3	3	60	THR	CA-CB-OG1	-5.44	97.57	109.00
1	1	193	LEU	CA-CB-CG	5.43	127.78	115.30
1	1	233	ASP	CB-CG-OD1	5.42	123.18	118.30
2	2	174	ASN	CA-C-N	5.42	127.04	116.20
1	1	270	ASN	O-C-N	5.40	131.35	122.70
4	4	44	SER	N-CA-CB	5.40	118.60	110.50
3	3	161	ILE	CA-CB-CG1	-5.40	100.75	111.00
2	2	44	ASP	CA-CB-CG	5.39	125.25	113.40
1	1	123	ARG	NH1-CZ-NH2	-5.38	113.48	119.40
3	3	115	LEU	CA-CB-CG	5.38	127.67	115.30
2	2	169	VAL	CB-CA-C	-5.38	101.18	111.40
3	3	231	THR	CA-CB-OG1	-5.36	97.74	109.00
1	1	202	ASP	CB-CA-C	5.35	121.10	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	244	TYR	CB-CG-CD2	-5.35	117.79	121.00
2	2	262	GLN	CA-C-O	-5.35	108.87	120.10
1	1	64	GLU	CA-CB-CG	5.34	125.15	113.40
3	3	65	ASN	N-CA-CB	-5.34	100.98	110.60
1	1	128	TYR	CB-CG-CD1	5.32	124.19	121.00
2	2	259	ILE	CB-CG1-CD1	-5.31	99.03	113.90
2	2	88	ASP	CA-CB-CG	-5.30	101.75	113.40
3	3	42	ASN	CB-CG-OD1	-5.28	111.03	121.60
3	3	116	MET	CB-CG-SD	-5.27	96.59	112.40
3	3	33	ARG	CB-CG-CD	-5.27	97.91	111.60
2	2	143	LYS	CD-CE-NZ	-5.26	99.59	111.70
1	1	242	ARG	CD-NE-CZ	-5.25	116.25	123.60
1	1	205	SER	O-C-N	5.24	131.08	122.70
2	2	38	TRP	CA-CB-CG	-5.24	103.75	113.70
3	3	74	ASN	OD1-CG-ND2	5.22	133.90	121.90
1	1	275	THR	CA-C-N	5.21	128.67	117.20
3	3	78	GLU	CA-CB-CG	5.21	124.87	113.40
1	1	271	TYR	CB-CG-CD2	-5.20	117.88	121.00
4	4	48	ASP	CA-CB-CG	-5.20	101.96	113.40
2	2	170	LEU	CB-CG-CD2	5.20	119.83	111.00
2	2	203	TYR	CZ-CE2-CD2	-5.19	115.13	119.80
3	3	222	MET	CB-CG-SD	-5.19	96.83	112.40
1	1	275	THR	CA-C-O	-5.19	109.21	120.10
2	2	219	SER	N-CA-CB	5.19	118.28	110.50
1	1	282	ARG	CG-CD-NE	-5.18	100.92	111.80
1	1	162	GLU	OE1-CD-OE2	5.18	129.51	123.30
4	4	36	ALA	C-N-CA	-5.18	108.76	121.70
2	2	11	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	1	21	ILE	CA-CB-CG1	-5.17	101.18	111.00
2	2	52	LYS	CA-C-N	5.15	128.53	117.20
4	4	31	TYR	CG-CD2-CE2	-5.15	117.18	121.30
1	1	50	SER	CA-C-N	5.14	128.52	117.20
2	2	14	GLN	OE1-CD-NE2	5.14	133.73	121.90
1	1	150	ALA	C-N-CA	-5.13	108.87	121.70
2	2	203	TYR	CG-CD2-CE2	5.10	125.38	121.30
2	2	221	MET	CA-CB-CG	-5.10	104.63	113.30
1	1	150	ALA	CA-C-N	-5.10	105.99	117.20
2	2	14	GLN	CA-CB-CG	-5.10	102.19	113.40
4	4	58	ASP	O-C-N	5.09	130.85	122.70
1	1	164	ASP	CB-CG-OD2	5.09	122.88	118.30
3	3	144	GLU	CA-CB-CG	5.07	124.56	113.40
2	2	18	LEU	CB-CA-C	5.06	119.82	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	274	ASN	CA-C-N	-5.06	106.06	117.20
3	3	141	ASP	CB-CG-OD1	5.05	122.85	118.30
1	1	121	TYR	CB-CG-CD2	5.05	124.03	121.00
1	1	17	THR	CA-CB-CG2	-5.04	105.34	112.40
3	3	86	PHE	CB-CA-C	5.04	120.48	110.40
2	2	170	LEU	CB-CA-C	5.04	119.77	110.20
3	3	172	GLN	CG-CD-NE2	5.03	128.77	116.70
4	4	39	SER	O-C-N	5.03	130.74	122.70
1	1	282	ARG	CB-CA-C	-5.02	100.35	110.40
1	1	270	ASN	CB-CA-C	-5.02	100.36	110.40
3	3	224	ASP	CB-CG-OD2	5.02	122.82	118.30
3	3	146	MET	CB-CA-C	5.01	120.42	110.40
3	3	187	LEU	N-CA-CB	-5.01	100.38	110.40
2	2	9	TYR	CA-CB-CG	-5.01	103.88	113.40
3	3	86	PHE	CG-CD1-CE1	5.01	126.31	120.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	219	SER	Mainchain
1	1	220	HIS	Mainchain
1	1	259	ARG	Sidechain
1	1	268	ARG	Sidechain
2	2	12	ARG	Sidechain
2	2	255	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2168	0	2103	175	0
2	2	1952	0	1926	126	0
3	3	1849	0	1831	149	0
4	4	297	0	294	36	0
5	1	26	0	27	7	0
All	All	6292	0	6181	411	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (411) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:57:ASN:CB	3:3:57:ASN:CA	1.75	1.58
4:4:33:LYS:CE	4:4:33:LYS:NZ	1.67	1.55
2:2:52:LYS:NZ	2:2:52:LYS:CE	1.68	1.54
1:1:285:ASP:CB	1:1:285:ASP:CA	1.80	1.54
1:1:220:HIS:C	1:1:221:MET:CA	1.94	1.33
1:1:220:HIS:CA	1:1:221:MET:N	1.94	1.29
1:1:220:HIS:O	1:1:221:MET:N	1.74	1.21
2:2:158:SER:OG	2:2:167:LYS:HE2	1.46	1.14
1:1:136:GLN:NE2	1:1:140:ALA:CB	2.17	1.07
3:3:21:SER:O	4:4:37:SER:HB2	1.54	1.07
1:1:285:ASP:CA	1:1:285:ASP:OD1	2.00	1.07
1:1:258:PRO:HG2	3:3:99:GLU:HG2	1.36	1.06
1:1:47:PRO:HA	3:3:164:THR:HG21	1.34	1.05
2:2:12:ARG:NH1	2:2:12:ARG:HG3	1.69	1.05
2:2:255:ARG:HG2	2:2:256:SER:H	1.24	1.03
1:1:282:ARG:HG3	3:3:57:ASN:HB3	1.42	1.02
3:3:179:ASP:HB3	3:3:182:THR:HG22	1.44	1.00
1:1:99:PHE:CD1	1:1:99:PHE:O	2.15	1.00
2:2:136:GLU:HB3	2:2:140:VAL:HG21	1.44	0.97
3:3:57:ASN:CB	3:3:57:ASN:N	2.28	0.97
1:1:136:GLN:NE2	1:1:140:ALA:HB1	1.80	0.96
1:1:58:MET:HE1	3:3:216:ASP:HA	1.49	0.95
1:1:83:GLN:HG3	1:1:85:LYS:HE2	1.47	0.94
2:2:41:TYR:CE2	2:2:55:LYS:HD3	2.05	0.92
3:3:57:ASN:CB	3:3:57:ASN:C	2.37	0.92
1:1:285:ASP:CB	1:1:285:ASP:N	2.34	0.91
3:3:179:ASP:HB3	3:3:182:THR:CG2	2.01	0.91
1:1:285:ASP:CA	1:1:285:ASP:CG	2.37	0.91
2:2:235:THR:HG23	2:2:236:PRO:HD2	1.53	0.91
2:2:12:ARG:HG3	2:2:12:ARG:HH11	1.28	0.91
1:1:28:THR:HB	1:1:30:LYS:H	1.35	0.90
2:2:11:ASP:HB2	4:4:68:ASN:OD1	1.71	0.90
1:1:285:ASP:CB	1:1:285:ASP:C	2.40	0.89
1:1:285:ASP:OD1	1:1:285:ASP:HA	1.73	0.88
3:3:198:PRO:HD2	3:3:201:THR:HG21	1.55	0.88
2:2:20:ASN:ND2	2:2:62:ARG:HE	1.72	0.87
1:1:47:PRO:HA	3:3:164:THR:CG2	2.03	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:77:VAL:C	1:1:109:LEU:HD12	1.95	0.86
2:2:195:ASN:ND2	2:2:196:THR:HG23	1.90	0.86
2:2:116:LYS:HB3	3:3:121:ALA:HB3	1.57	0.85
2:2:12:ARG:HH11	2:2:12:ARG:CG	1.89	0.85
3:3:57:ASN:CA	3:3:57:ASN:CG	2.45	0.84
1:1:90:ILE:HD13	1:1:90:ILE:N	1.92	0.84
1:1:282:ARG:HD2	1:1:285:ASP:O	1.78	0.84
2:2:158:SER:OG	2:2:167:LYS:CE	2.27	0.82
1:1:220:HIS:O	1:1:221:MET:CA	2.18	0.82
2:2:10:SER:OG	2:2:12:ARG:HB2	1.78	0.82
2:2:30:ASN:HD22	2:2:31:ALA:H	1.27	0.82
2:2:52:LYS:NZ	2:2:52:LYS:CD	2.43	0.82
1:1:248:LYS:HE3	4:4:38:THR:O	1.80	0.82
2:2:136:GLU:CB	2:2:140:VAL:HG21	2.09	0.82
4:4:59:LEU:HD21	4:4:61:LEU:HD13	1.61	0.81
1:1:220:HIS:C	1:1:221:MET:N	0.76	0.81
2:2:9:TYR:HD1	2:2:9:TYR:N	1.77	0.80
1:1:58:MET:CE	3:3:216:ASP:HA	2.11	0.80
2:2:195:ASN:HD22	2:2:196:THR:HG23	1.47	0.79
4:4:68:ASN:OD1	4:4:68:ASN:N	2.11	0.79
2:2:9:TYR:N	2:2:9:TYR:CD1	2.43	0.79
1:1:142:TYR:O	1:1:142:TYR:CD1	2.36	0.78
1:1:58:MET:HE1	3:3:216:ASP:CA	2.13	0.78
1:1:220:HIS:O	1:1:221:MET:HA	1.83	0.77
1:1:208:ASP:HB3	1:1:211:THR:CG2	2.13	0.77
1:1:282:ARG:HG3	3:3:57:ASN:CB	2.15	0.77
1:1:94:ARG:CZ	1:1:101:ASP:OD1	2.33	0.77
1:1:188:VAL:HG21	5:1:290:W84:H2C2	1.66	0.77
2:2:255:ARG:HG2	2:2:256:SER:N	2.00	0.77
3:3:79:GLN:HB2	3:3:190:TRP:CZ3	2.19	0.76
1:1:94:ARG:NH1	1:1:94:ARG:HG2	2.00	0.75
1:1:270:ASN:HA	2:2:133:ALA:HB1	1.68	0.75
1:1:208:ASP:HB3	1:1:211:THR:HG22	1.68	0.74
3:3:197:LEU:HB3	3:3:201:THR:CG2	2.18	0.74
4:4:43:GLN:HG2	4:4:45:LEU:HB2	1.70	0.73
3:3:26:PRO:O	3:3:27:ASN:HB2	1.89	0.73
2:2:188:PHE:O	2:2:194:ASN:ND2	2.22	0.73
2:2:262:GLN:HE21	2:2:262:GLN:C	1.91	0.73
1:1:92:ASN:OD1	1:1:95:GLU:HB2	1.87	0.73
1:1:282:ARG:CG	3:3:57:ASN:HB3	2.18	0.73
1:1:47:PRO:CA	3:3:164:THR:HG21	2.15	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:53:THR:HG22	2:2:252:SER:HB2	1.71	0.72
1:1:94:ARG:NH2	1:1:101:ASP:OD1	2.23	0.71
1:1:201:TYR:HD2	1:1:214:GLY:O	1.73	0.71
1:1:258:PRO:CG	3:3:99:GLU:HG2	2.16	0.71
2:2:20:ASN:HD21	2:2:62:ARG:HE	1.39	0.71
4:4:33:LYS:NZ	4:4:33:LYS:CD	2.52	0.71
2:2:230:VAL:CG2	2:2:234:ALA:HB3	2.20	0.71
1:1:19:ALA:HB2	1:1:58:MET:HG2	1.72	0.71
1:1:105:ASN:HD21	1:1:108:SER:HB2	1.56	0.70
3:3:57:ASN:CA	3:3:57:ASN:OD1	2.38	0.70
2:2:174:ASN:C	2:2:174:ASN:HD22	1.93	0.70
1:1:99:PHE:O	1:1:99:PHE:CG	2.43	0.70
2:2:235:THR:CG2	2:2:236:PRO:HD2	2.21	0.69
2:2:136:GLU:HB3	2:2:140:VAL:CG2	2.21	0.69
2:2:230:VAL:HG23	2:2:234:ALA:HB3	1.74	0.69
3:3:98:GLY:O	3:3:102:GLN:HG3	1.92	0.69
1:1:82:ILE:HG22	1:1:100:ASN:H	1.57	0.69
1:1:89:GLY:C	1:1:90:ILE:HD13	2.13	0.68
1:1:136:GLN:HE21	1:1:235:HIS:CG	2.10	0.68
3:3:20:GLN:HE22	4:4:31:TYR:H	1.42	0.68
4:4:29:ILE:HG22	4:4:29:ILE:O	1.94	0.68
1:1:83:GLN:CG	1:1:85:LYS:HE2	2.24	0.67
1:1:136:GLN:CD	1:1:140:ALA:CB	2.63	0.67
1:1:278:VAL:HG12	3:3:62:ASP:OD2	1.95	0.67
3:3:61:LYS:HD3	3:3:63:GLU:OE2	1.95	0.67
1:1:99:PHE:CD1	1:1:99:PHE:C	2.68	0.67
2:2:84:ASP:OD1	2:2:87:LYS:HE2	1.94	0.67
1:1:152:TYR:O	1:1:154:PRO:HD3	1.94	0.67
1:1:142:TYR:CD1	1:1:142:TYR:C	2.68	0.66
2:2:195:ASN:HD22	2:2:195:ASN:C	1.99	0.66
1:1:136:GLN:NE2	1:1:235:HIS:CD2	2.63	0.66
3:3:89:ASP:HA	3:3:93:LYS:HD2	1.78	0.66
1:1:107:SER:HB3	1:1:113:ARG:HD2	1.77	0.66
3:3:42:ASN:HD22	3:3:44:LEU:H	1.43	0.66
3:3:197:LEU:HB3	3:3:201:THR:HG22	1.77	0.66
1:1:285:ASP:CB	1:1:285:ASP:H	2.08	0.65
2:2:190:ASN:HD21	3:3:118:THR:HA	1.62	0.65
2:2:256:SER:O	2:2:257:LYS:HB3	1.96	0.65
2:2:149:PRO:HG3	2:2:154:ILE:HG13	1.78	0.64
2:2:205:ASN:HD22	2:2:206:SER:H	1.45	0.64
2:2:12:ARG:HH21	3:3:157:LEU:HD21	1.63	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:79:GLN:HB2	3:3:190:TRP:CE3	2.32	0.64
2:2:30:ASN:HD22	2:2:31:ALA:N	1.94	0.64
2:2:23:ILE:HD11	2:2:243:THR:HG21	1.79	0.64
2:2:12:ARG:NH1	4:4:68:ASN:O	2.31	0.64
1:1:60:PHE:CE2	3:3:218:LYS:HB3	2.33	0.64
3:3:179:ASP:OD1	3:3:180:THR:N	2.32	0.63
2:2:205:ASN:ND2	2:2:206:SER:H	1.97	0.63
2:2:187:GLN:HE21	2:2:197:ALA:HA	1.63	0.63
1:1:87:ALA:HA	1:1:90:ILE:HG12	1.80	0.63
2:2:155:ASP:C	2:2:155:ASP:OD1	2.37	0.62
3:3:75:ARG:O	3:3:194:SER:HB2	1.99	0.62
1:1:136:GLN:NE2	1:1:235:HIS:CG	2.67	0.62
2:2:40:GLU:HG3	2:2:41:TYR:O	2.00	0.62
3:3:84:ASN:ND2	3:3:86:PHE:H	1.98	0.62
1:1:136:GLN:HE22	1:1:140:ALA:HB1	1.65	0.61
2:2:13:VAL:O	2:2:14:GLN:HG2	1.99	0.61
1:1:188:VAL:HG11	5:1:290:W84:H3C1	1.82	0.61
2:2:38:TRP:CZ3	4:4:57:LYS:HD2	2.36	0.61
2:2:133:ALA:O	2:2:166:VAL:HG12	2.01	0.61
3:3:57:ASN:ND2	3:3:91:VAL:HG13	2.15	0.61
1:1:187:SER:HB3	3:3:21:SER:CB	2.31	0.61
1:1:281:LYS:HD2	3:3:59:HIS:O	2.01	0.61
1:1:215:ILE:O	1:1:218:LEU:N	2.30	0.61
3:3:55:MET:HG3	3:3:55:MET:O	1.99	0.61
1:1:90:ILE:N	1:1:90:ILE:CD1	2.62	0.60
3:3:56:ASN:HB3	3:3:66:SER:HA	1.83	0.60
3:3:76:GLN:O	3:3:78:GLU:N	2.34	0.60
1:1:265:SER:HB3	1:1:268:ARG:HG2	1.83	0.60
3:3:179:ASP:CB	3:3:182:THR:HG22	2.26	0.60
1:1:51:ILE:HD13	3:3:166:PRO:HG3	1.82	0.59
1:1:77:VAL:C	1:1:109:LEU:CD1	2.69	0.59
3:3:131:TYR:HB3	3:3:149:THR:HB	1.82	0.59
1:1:58:MET:HE1	3:3:216:ASP:C	2.23	0.59
1:1:259:ARG:HD2	1:1:263:TYR:CE1	2.38	0.59
2:2:256:SER:O	2:2:257:LYS:CB	2.50	0.59
1:1:94:ARG:NH1	1:1:94:ARG:CG	2.60	0.59
3:3:84:ASN:HD22	3:3:86:PHE:H	1.49	0.59
1:1:188:VAL:HG21	5:1:290:W84:C2C	2.33	0.58
2:2:11:ASP:H	4:4:68:ASN:CG	2.06	0.58
2:2:30:ASN:HD21	4:4:58:ASP:H	1.51	0.58
3:3:180:THR:O	3:3:183:SER:HB3	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:179:ASP:HB3	3:3:182:THR:HB	1.85	0.58
1:1:136:GLN:NE2	1:1:140:ALA:HB2	2.15	0.58
1:1:151:MET:SD	1:1:170:SER:HB2	2.43	0.58
2:2:177:LEU:HD11	3:3:94:THR:HG21	1.86	0.58
3:3:175:TYR:HD2	3:3:182:THR:HG21	1.68	0.57
2:2:64:TYR:CD1	2:2:89:MET:HB3	2.39	0.57
2:2:204:ILE:HG12	3:3:37:PRO:HG2	1.87	0.57
1:1:285:ASP:HB3	1:1:287:LYS:N	2.18	0.57
2:2:52:LYS:NZ	2:2:52:LYS:HD3	2.20	0.57
1:1:188:VAL:HG21	5:1:290:W84:H3C1	1.86	0.57
1:1:43:MET:HG3	1:1:44:PRO:HD2	1.87	0.56
1:1:102:TRP:O	1:1:223:SER:HB2	2.05	0.56
1:1:136:GLN:CD	1:1:140:ALA:HB3	2.23	0.56
3:3:31:THR:CG2	3:3:32:PRO:HD2	2.34	0.56
1:1:85:LYS:HB3	1:1:236:LYS:HG3	1.87	0.56
1:1:176:VAL:HG22	5:1:290:W84:H312	1.87	0.56
2:2:10:SER:OG	2:2:12:ARG:CB	2.53	0.56
3:3:53:ILE:HD11	3:3:211:ILE:HB	1.87	0.56
1:1:236:LYS:HE3	1:1:238:LEU:HD13	1.88	0.55
2:2:189:ILE:HA	2:2:194:ASN:ND2	2.21	0.55
4:4:43:GLN:O	4:4:45:LEU:HB3	2.05	0.55
1:1:38:GLU:CD	3:3:116:MET:HE1	2.27	0.55
2:2:77:GLY:O	2:2:156:LEU:HB2	2.07	0.55
2:2:235:THR:HG22	2:2:236:PRO:N	2.22	0.55
1:1:138:ASP:O	1:1:139:SER:C	2.44	0.55
1:1:228:ILE:HD11	1:1:239:VAL:HG21	1.88	0.55
2:2:230:VAL:HG23	2:2:231:PRO:O	2.05	0.55
2:2:38:TRP:CD1	2:2:39:PRO:HD2	2.42	0.55
3:3:199:PRO:O	3:3:200:GLU:HB2	2.05	0.55
1:1:79:VAL:HG22	1:1:242:ARG:HG2	1.89	0.54
1:1:266:ILE:HD12	3:3:235:THR:HA	1.88	0.54
3:3:31:THR:HG23	3:3:32:PRO:HD2	1.87	0.54
3:3:198:PRO:O	3:3:201:THR:HB	2.07	0.54
4:4:59:LEU:HD21	4:4:61:LEU:CD1	2.34	0.54
2:2:230:VAL:HB	2:2:231:PRO:HD2	1.89	0.54
3:3:20:GLN:HE22	4:4:31:TYR:N	2.04	0.54
2:2:38:TRP:HZ3	4:4:57:LYS:HD2	1.70	0.54
1:1:35:THR:HG23	3:3:160:THR:HB	1.90	0.54
2:2:170:LEU:CD2	3:3:64:VAL:HA	2.38	0.54
3:3:193:THR:O	3:3:194:SER:CB	2.55	0.54
3:3:55:MET:HA	3:3:91:VAL:HG11	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:117:TYR:CD1	3:3:155:ILE:HD13	2.43	0.54
3:3:197:LEU:HB3	3:3:201:THR:HG21	1.87	0.53
3:3:175:TYR:CD2	3:3:182:THR:HG21	2.43	0.53
1:1:271:TYR:HB2	1:1:272:PRO:HD2	1.89	0.53
2:2:235:THR:CG2	2:2:236:PRO:CD	2.86	0.53
3:3:18:ASP:OD2	4:4:40:SER:HB2	2.09	0.53
2:2:12:ARG:NH2	3:3:157:LEU:HD21	2.24	0.53
3:3:57:ASN:HB3	3:3:57:ASN:C	2.27	0.53
1:1:88:THR:O	1:1:90:ILE:HD13	2.09	0.52
1:1:83:GLN:HG3	1:1:85:LYS:CE	2.31	0.52
1:1:188:VAL:HG21	5:1:290:W84:C3C	2.39	0.52
1:1:88:THR:O	1:1:90:ILE:CD1	2.58	0.52
1:1:276:GLU:HB3	1:1:277:PRO:CD	2.39	0.52
1:1:77:VAL:O	1:1:109:LEU:HD12	2.07	0.52
1:1:187:SER:HB3	3:3:21:SER:HB2	1.92	0.52
3:3:216:ASP:O	3:3:218:LYS:HE3	2.09	0.52
1:1:136:GLN:HE21	1:1:235:HIS:CD2	2.28	0.52
1:1:236:LYS:NZ	1:1:238:LEU:HD11	2.25	0.52
2:2:174:ASN:C	2:2:174:ASN:ND2	2.63	0.52
1:1:103:LYS:O	1:1:104:ILE:C	2.49	0.52
1:1:43:MET:HE3	1:1:43:MET:HA	1.92	0.52
1:1:122:VAL:HG13	1:1:124:PHE:CE2	2.45	0.52
2:2:177:LEU:CD1	3:3:94:THR:HG21	2.40	0.52
1:1:219:SER:O	1:1:219:SER:OG	2.19	0.51
3:3:75:ARG:NH1	3:3:78:GLU:OE2	2.41	0.51
1:1:236:LYS:HE3	1:1:238:LEU:CD1	2.40	0.51
1:1:273:LYS:O	1:1:274:ASN:O	2.28	0.51
2:2:34:CYS:HB2	2:2:202:PRO:CD	2.41	0.51
3:3:193:THR:O	3:3:194:SER:HB3	2.08	0.51
3:3:214:CYS:HB3	3:3:215:PRO:HD2	1.92	0.51
4:4:44:SER:O	4:4:45:LEU:C	2.48	0.51
1:1:265:SER:HB2	2:2:138:GLY:O	2.11	0.51
3:3:101:VAL:HG13	3:3:176:THR:CG2	2.41	0.51
3:3:210:PHE:N	3:3:210:PHE:CD1	2.77	0.51
3:3:84:ASN:HD22	3:3:86:PHE:N	2.08	0.51
1:1:94:ARG:CG	1:1:94:ARG:HH11	2.24	0.50
1:1:114:LYS:NZ	3:3:99:GLU:OE2	2.44	0.50
1:1:65:THR:HG22	3:3:104:TYR:CZ	2.46	0.50
2:2:255:ARG:CG	2:2:256:SER:H	2.00	0.50
2:2:139:ASN:N	2:2:139:ASN:OD1	2.44	0.50
2:2:171:TYR:HA	2:2:176:THR:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:58:MET:CE	3:3:216:ASP:O	2.60	0.50
1:1:60:PHE:CD2	3:3:218:LYS:HB3	2.46	0.50
2:2:158:SER:HG	2:2:167:LYS:HE2	1.71	0.50
1:1:58:MET:HE1	3:3:216:ASP:O	2.12	0.50
2:2:8:GLY:C	2:2:9:TYR:HD1	2.14	0.50
2:2:143:LYS:HG2	2:2:163:GLY:O	2.12	0.49
3:3:63:GLU:C	3:3:65:ASN:H	2.14	0.49
1:1:58:MET:O	1:1:59:HIS:HB2	2.13	0.49
2:2:205:ASN:HD22	2:2:206:SER:N	2.09	0.49
2:2:19:GLY:HA2	2:2:58:THR:HG22	1.94	0.49
3:3:95:THR:O	3:3:99:GLU:HB2	2.13	0.49
2:2:34:CYS:HB2	2:2:202:PRO:HD2	1.94	0.49
3:3:20:GLN:NE2	4:4:31:TYR:H	2.11	0.49
1:1:273:LYS:O	1:1:274:ASN:C	2.52	0.48
2:2:30:ASN:ND2	2:2:31:ALA:H	2.05	0.48
1:1:82:ILE:CG2	1:1:100:ASN:H	2.23	0.48
3:3:125:ALA:HB3	3:3:155:ILE:HD12	1.95	0.48
3:3:129:LEU:O	3:3:150:HIS:HA	2.13	0.48
3:3:54:PRO:O	3:3:91:VAL:HG12	2.13	0.48
4:4:59:LEU:HG	4:4:60:MET:N	2.27	0.48
2:2:170:LEU:HD21	3:3:64:VAL:HA	1.94	0.48
2:2:135:HIS:CD2	2:2:160:ASN:HB3	2.49	0.48
2:2:10:SER:CB	4:4:68:ASN:OXT	2.61	0.48
1:1:280:LYS:HE3	3:3:89:ASP:OD1	2.13	0.48
3:3:115:LEU:HD22	3:3:129:LEU:HD21	1.95	0.48
3:3:190:TRP:CD1	3:3:190:TRP:N	2.81	0.48
1:1:122:VAL:O	1:1:197:TYR:HB2	2.13	0.48
3:3:20:GLN:HE22	4:4:30:ASN:HA	1.78	0.48
1:1:158:PRO:HB2	1:1:167:THR:HG22	1.96	0.48
3:3:61:LYS:O	3:3:61:LYS:HG2	2.07	0.48
3:3:112:ARG:NH1	3:3:112:ARG:HG2	2.27	0.48
3:3:175:TYR:H	3:3:182:THR:HG21	1.78	0.48
1:1:87:ALA:CA	1:1:90:ILE:HG12	2.44	0.47
1:1:146:LEU:HD13	1:1:228:ILE:HD13	1.95	0.47
3:3:112:ARG:HD3	3:3:162:VAL:CG1	2.44	0.47
1:1:104:ILE:HG13	1:1:223:SER:HA	1.96	0.47
1:1:134:ALA:HB2	1:1:180:VAL:HG11	1.95	0.47
1:1:268:ARG:CZ	2:2:139:ASN:HB2	2.44	0.47
2:2:177:LEU:CD1	3:3:94:THR:CG2	2.93	0.47
4:4:29:ILE:O	4:4:29:ILE:CG2	2.62	0.47
1:1:83:GLN:OE1	1:1:236:LYS:HD2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:165:ASP:HB3	1:1:167:THR:H	1.79	0.47
1:1:206:HIS:ND1	1:1:206:HIS:N	2.62	0.47
2:2:13:VAL:HA	2:2:25:THR:O	2.15	0.47
2:2:63:PHE:CD1	2:2:245:ALA:HB2	2.50	0.47
4:4:44:SER:C	4:4:46:SER:N	2.68	0.47
1:1:188:VAL:CG2	5:1:290:W84:H2C2	2.40	0.47
2:2:195:ASN:ND2	2:2:195:ASN:C	2.66	0.47
1:1:129:THR:OG1	1:1:185:ARG:NH1	2.43	0.46
3:3:84:ASN:ND2	3:3:84:ASN:C	2.69	0.46
1:1:110:VAL:O	1:1:111:GLN:C	2.53	0.46
1:1:74:ALA:HB3	3:3:15:THR:HB	1.97	0.46
1:1:92:ASN:C	1:1:92:ASN:ND2	2.67	0.46
2:2:130:HIS:ND1	2:2:219:SER:OG	2.47	0.46
2:2:170:LEU:HD23	3:3:64:VAL:CG2	2.45	0.46
4:4:61:LEU:HD12	4:4:61:LEU:HA	1.63	0.46
1:1:236:LYS:HE2	1:1:236:LYS:HB3	1.83	0.46
1:1:92:ASN:CG	1:1:95:GLU:HB2	2.36	0.46
2:2:156:LEU:HD11	2:2:173:MET:SD	2.56	0.46
2:2:158:SER:HG	2:2:167:LYS:CE	2.26	0.46
3:3:101:VAL:HG22	3:3:219:LEU:HD11	1.98	0.46
1:1:138:ASP:O	1:1:139:SER:O	2.33	0.46
2:2:148:HIS:N	2:2:149:PRO:CD	2.79	0.46
3:3:55:MET:CE	3:3:91:VAL:HG21	2.46	0.46
3:3:57:ASN:CB	3:3:57:ASN:H	2.26	0.45
2:2:228:LEU:CD1	2:2:238:LEU:HD22	2.47	0.45
1:1:77:VAL:CA	1:1:109:LEU:HD12	2.46	0.45
2:2:190:ASN:H	2:2:194:ASN:CB	2.30	0.45
4:4:30:ASN:HA	4:4:30:ASN:HD22	1.40	0.45
1:1:31:VAL:HG11	1:1:34:LEU:HD12	1.98	0.45
1:1:132:ALA:O	1:1:181:GLY:N	2.39	0.45
2:2:170:LEU:HD23	3:3:64:VAL:HG22	1.99	0.45
2:2:187:GLN:NE2	2:2:198:THR:H	2.14	0.45
3:3:50:ASP:HA	3:3:212:SER:HB3	1.98	0.45
3:3:84:ASN:HD22	3:3:84:ASN:C	2.20	0.45
1:1:152:TYR:O	1:1:173:ASN:ND2	2.50	0.45
2:2:91:VAL:HG12	2:2:95:ASN:HD22	1.82	0.45
3:3:192:GLN:HE21	3:3:192:GLN:HA	1.81	0.45
1:1:28:THR:HG22	1:1:29:GLN:H	1.81	0.45
1:1:64:GLU:O	1:1:64:GLU:HG2	2.17	0.45
2:2:13:VAL:C	2:2:14:GLN:CG	2.85	0.45
2:2:37:GLU:CD	3:3:35:HIS:HE2	2.19	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:235:THR:CG2	2:2:236:PRO:N	2.79	0.45
3:3:179:ASP:HB3	3:3:182:THR:CB	2.45	0.45
1:1:43:MET:HA	1:1:43:MET:CE	2.46	0.45
2:2:190:ASN:H	2:2:194:ASN:HB3	1.82	0.45
2:2:259:ILE:HG21	2:2:259:ILE:HD13	1.74	0.45
1:1:198:ASN:HB3	1:1:200:PHE:O	2.17	0.44
3:3:57:ASN:N	3:3:57:ASN:HB2	2.25	0.44
1:1:142:TYR:HE1	1:1:144:SER:OG	2.00	0.44
1:1:268:ARG:NH1	3:3:236:GLU:O	2.46	0.44
1:1:285:ASP:HB3	1:1:288:SER:H	1.82	0.44
1:1:289:TYR:CE2	3:3:138:GLY:HA3	2.53	0.44
3:3:61:LYS:O	3:3:63:GLU:HG3	2.17	0.44
1:1:207:ASP:HA	2:2:144:TYR:CE2	2.52	0.44
3:3:116:MET:HG3	3:3:159:SER:OG	2.17	0.44
4:4:59:LEU:CD2	4:4:61:LEU:HD13	2.41	0.44
4:4:43:GLN:O	4:4:45:LEU:CB	2.66	0.44
3:3:55:MET:HE2	3:3:91:VAL:HG21	1.99	0.44
3:3:181:TYR:CD1	3:3:181:TYR:C	2.91	0.44
3:3:197:LEU:HD21	3:3:205:VAL:HG11	1.99	0.44
1:1:282:ARG:CG	3:3:57:ASN:CB	2.89	0.44
1:1:289:TYR:CD2	3:3:138:GLY:HA3	2.52	0.44
2:2:146:PHE:CG	2:2:164:GLY:HA2	2.52	0.44
1:1:286:ILE:HG23	3:3:81:PHE:HA	2.00	0.44
3:3:101:VAL:HG13	3:3:176:THR:HG22	1.99	0.44
4:4:43:GLN:HG3	4:4:45:LEU:H	1.82	0.44
1:1:47:PRO:HB3	3:3:166:PRO:HB3	1.99	0.43
3:3:208:LEU:HA	3:3:208:LEU:HD12	1.73	0.43
1:1:87:ALA:HB2	1:1:98:LEU:CD1	2.48	0.43
1:1:82:ILE:HG22	1:1:100:ASN:HB2	2.00	0.43
1:1:159:ASN:HA	1:1:160:PRO:HD3	1.65	0.43
2:2:262:GLN:C	2:2:262:GLN:NE2	2.66	0.43
3:3:57:ASN:HD21	3:3:91:VAL:HG13	1.84	0.43
1:1:142:TYR:C	1:1:142:TYR:HD1	2.18	0.43
2:2:10:SER:CB	2:2:12:ARG:HB2	2.48	0.43
2:2:91:VAL:HG12	2:2:95:ASN:ND2	2.34	0.43
3:3:112:ARG:HG2	3:3:112:ARG:HH11	1.83	0.43
3:3:61:LYS:HG2	3:3:63:GLU:HG3	2.00	0.43
2:2:70:THR:HG22	2:2:72:THR:HG22	2.01	0.43
2:2:95:ASN:HB3	2:2:251:PHE:CE2	2.53	0.43
2:2:205:ASN:ND2	2:2:206:SER:N	2.66	0.43
3:3:151:VAL:HG11	3:3:161:ILE:HD11	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:98:LEU:HD23	1:1:98:LEU:HA	1.82	0.42
3:3:195:LEU:C	3:3:196:ILE:HG12	2.40	0.42
2:2:13:VAL:C	2:2:14:GLN:HG2	2.39	0.42
1:1:87:ALA:HB2	1:1:98:LEU:HD11	2.02	0.42
1:1:206:HIS:NE2	1:1:208:ASP:HB2	2.34	0.42
1:1:187:SER:HB3	3:3:21:SER:HB3	2.01	0.42
2:2:10:SER:OG	4:4:68:ASN:OXT	2.35	0.42
3:3:226:GLN:HE21	3:3:226:GLN:HB2	1.21	0.42
1:1:137:PRO:HG3	1:1:238:LEU:HD22	2.00	0.42
2:2:225:ILE:O	3:3:68:LEU:HD21	2.19	0.42
2:2:228:LEU:HD11	2:2:238:LEU:HD22	2.02	0.42
2:2:40:GLU:O	2:2:40:GLU:CG	2.61	0.42
2:2:122:LEU:HD23	2:2:224:PRO:HA	2.02	0.42
4:4:43:GLN:O	4:4:44:SER:C	2.58	0.42
1:1:201:TYR:H	2:2:131:GLN:HE21	1.68	0.42
1:1:285:ASP:HB3	1:1:288:SER:N	2.34	0.42
3:3:44:LEU:HA	3:3:44:LEU:HD23	1.79	0.42
1:1:93:HIS:CE1	1:1:163:TRP:HD1	2.38	0.42
1:1:289:TYR:CZ	3:3:139:PRO:HD2	2.55	0.42
1:1:261:LEU:HD11	2:2:171:TYR:CD2	2.55	0.42
1:1:286:ILE:HD13	1:1:286:ILE:HG21	1.77	0.41
2:2:69:LYS:O	2:2:239:PRO:HA	2.20	0.41
4:4:43:GLN:HG2	4:4:43:GLN:O	2.18	0.41
1:1:86:ASP:OD1	1:1:88:THR:HB	2.20	0.41
3:3:47:ILE:HG21	3:3:47:ILE:HD13	1.51	0.41
3:3:113:PHE:CE2	3:3:115:LEU:HD13	2.56	0.41
2:2:235:THR:HG22	2:2:237:SER:N	2.35	0.41
3:3:167:TRP:HZ2	3:3:172:GLN:HA	1.86	0.41
3:3:18:ASP:CG	4:4:40:SER:HB2	2.41	0.41
1:1:98:LEU:O	1:1:99:PHE:HB3	2.19	0.41
2:2:43:PRO:HG2	2:2:46:ASP:HB2	2.03	0.41
3:3:137:ARG:HH11	3:3:137:ARG:HD3	1.22	0.41
1:1:38:GLU:CD	3:3:116:MET:CE	2.88	0.41
1:1:54:ARG:HH11	1:1:54:ARG:HD2	1.55	0.41
1:1:165:ASP:CB	1:1:167:THR:OG1	2.69	0.41
2:2:84:ASP:HB2	2:2:216:ASN:HD21	1.86	0.41
3:3:179:ASP:CB	3:3:182:THR:CG2	2.88	0.41
1:1:78:HIS:NE2	1:1:80:THR:HB	2.36	0.41
3:3:64:VAL:HG12	3:3:64:VAL:O	2.21	0.41
3:3:157:LEU:HD23	3:3:157:LEU:O	2.21	0.41
2:2:13:VAL:HG22	2:2:26:GLN:HA	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:20:GLN:NE2	4:4:30:ASN:HA	2.36	0.40
1:1:265:SER:OG	2:2:139:ASN:HB3	2.21	0.40
3:3:214:CYS:HB3	3:3:215:PRO:CD	2.51	0.40
1:1:208:ASP:HB3	1:1:211:THR:HB	2.04	0.40
1:1:228:ILE:HD11	1:1:239:VAL:CG2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	271/289 (94%)	251 (93%)	16 (6%)	4 (2%)	10 42
2	2	253/262 (97%)	233 (92%)	18 (7%)	2 (1%)	19 57
3	3	234/236 (99%)	216 (92%)	15 (6%)	3 (1%)	12 45
4	4	38/68 (56%)	34 (90%)	3 (8%)	1 (3%)	5 27
All	All	796/855 (93%)	734 (92%)	52 (6%)	10 (1%)	12 45

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	3	57	ASN
3	3	77	ASN
1	1	99	PHE
1	1	139	SER
1	1	165	ASP
2	2	255	ARG
2	2	257	LYS
4	4	47	MET
1	1	104	ILE
3	3	178	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	239/253 (94%)	191 (80%)	48 (20%)	1 6
2	2	223/229 (97%)	179 (80%)	44 (20%)	1 7
3	3	209/209 (100%)	171 (82%)	38 (18%)	1 9
4	4	33/57 (58%)	20 (61%)	13 (39%)	0 0
All	All	704/748 (94%)	561 (80%)	143 (20%)	1 6

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	18	VAL
1	1	21	ILE
1	1	22	SER
1	1	23	SER
1	1	28	THR
1	1	29	GLN
1	1	30	LYS
1	1	38	GLU
1	1	43	MET
1	1	47	PRO
1	1	63	SER
1	1	81	GLU
1	1	90	ILE
1	1	97	LYS
1	1	99	PHE
1	1	100	ASN
1	1	101	ASP
1	1	103	LYS
1	1	105	ASN
1	1	107	SER
1	1	122	VAL
1	1	138	ASP
1	1	142	TYR
1	1	143	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	144	SER
1	1	145	ASN
1	1	159	ASN
1	1	161	LYS
1	1	165	ASP
1	1	170	SER
1	1	172	SER
1	1	173	ASN
1	1	176	VAL
1	1	183	THR
1	1	184	SER
1	1	185	ARG
1	1	187	SER
1	1	202	ASP
1	1	215	ILE
1	1	216	THR
1	1	217	VAL
1	1	220	HIS
1	1	240	LYS
1	1	256	ARG
1	1	268	ARG
1	1	274	ASN
1	1	278	VAL
1	1	287	LYS
2	2	11	ASP
2	2	12	ARG
2	2	20	ASN
2	2	26	GLN
2	2	30	ASN
2	2	49	ASP
2	2	52	LYS
2	2	66	LEU
2	2	69	LYS
2	2	73	THR
2	2	76	LYS
2	2	81	LYS
2	2	87	LYS
2	2	88	ASP
2	2	103	ARG
2	2	116	LYS
2	2	119	SER
2	2	136	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	141	SER
2	2	145	THR
2	2	152	ARG
2	2	165	PRO
2	2	168	ASP
2	2	169	VAL
2	2	170	LEU
2	2	174	ASN
2	2	187	GLN
2	2	192	ARG
2	2	195	ASN
2	2	205	ASN
2	2	209	ILE
2	2	211	SER
2	2	217	ASN
2	2	221	MET
2	2	225	ILE
2	2	232	THR
2	2	236	PRO
2	2	238	LEU
2	2	247	MET
2	2	250	GLU
2	2	254	ILE
2	2	255	ARG
2	2	256	SER
2	2	262	GLN
3	3	16	THR
3	3	33	ARG
3	3	46	ILE
3	3	55	MET
3	3	56	ASN
3	3	60	THR
3	3	61	LYS
3	3	65	ASN
3	3	84	ASN
3	3	91	VAL
3	3	94	THR
3	3	101	VAL
3	3	112	ARG
3	3	114	SER
3	3	115	LEU
3	3	137	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	3	146	MET
3	3	157	LEU
3	3	158	GLN
3	3	159	SER
3	3	164	THR
3	3	172	GLN
3	3	174	ARG
3	3	182	THR
3	3	192	GLN
3	3	194	SER
3	3	196	ILE
3	3	201	THR
3	3	208	LEU
3	3	211	ILE
3	3	217	PHE
3	3	218	LYS
3	3	219	LEU
3	3	220	ARG
3	3	223	LYS
3	3	226	GLN
3	3	228	ILE
3	3	230	GLN
4	4	29	ILE
4	4	33	LYS
4	4	40	SER
4	4	43	GLN
4	4	45	LEU
4	4	46	SER
4	4	47	MET
4	4	50	SER
4	4	51	LYS
4	4	59	LEU
4	4	61	LEU
4	4	67	LEU
4	4	68	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	61	ASN
1	1	92	ASN
1	1	100	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	136	GLN
1	1	173	ASN
1	1	198	ASN
1	1	235	HIS
2	2	15	GLN
2	2	20	ASN
2	2	30	ASN
2	2	131	GLN
2	2	174	ASN
2	2	187	GLN
2	2	190	ASN
2	2	195	ASN
2	2	205	ASN
2	2	216	ASN
2	2	217	ASN
2	2	262	GLN
3	3	20	GLN
3	3	41	HIS
3	3	42	ASN
3	3	56	ASN
3	3	84	ASN
3	3	102	GLN
3	3	140	GLN
3	3	192	GLN
3	3	226	GLN
4	4	30	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	W84	1	290	-	25,28,28	3.05	6 (24%)	31,36,36	2.83	8 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	W84	1	290	-	-	5/14/24/24	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	290	W84	C2A-N3A	10.92	1.43	1.27
5	1	290	W84	C4A-N3A	-7.32	1.35	1.48
5	1	290	W84	O1A-C2A	-4.18	1.29	1.36
5	1	290	W84	C4-C5	-3.90	1.34	1.39
5	1	290	W84	O1A-C5A	-3.77	1.38	1.45
5	1	290	W84	O1B-C7C	2.61	1.52	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	1	290	W84	CM1-C4A-N3A	7.78	133.42	111.63
5	1	290	W84	O1A-C2A-N3A	-7.71	110.16	118.17
5	1	290	W84	O1A-C2A-C4B	6.22	124.09	115.85
5	1	290	W84	O1A-C5A-C4A	5.38	111.47	104.94
5	1	290	W84	C4A-N3A-C2A	4.90	113.05	106.44
5	1	290	W84	C5A-C4A-N3A	-3.85	98.51	103.70
5	1	290	W84	CM1-C4A-C5A	-2.53	104.69	113.99
5	1	290	W84	C1C-C5-C4	2.52	135.14	128.60

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1	290	W84	C3C-C4C-C5C-C6C
5	1	290	W84	C1C-C2C-C3C-C4C
5	1	290	W84	C2C-C1C-C5-C4
5	1	290	W84	C5-C1C-C2C-C3C
5	1	290	W84	C6C-C7C-O1B-C1B

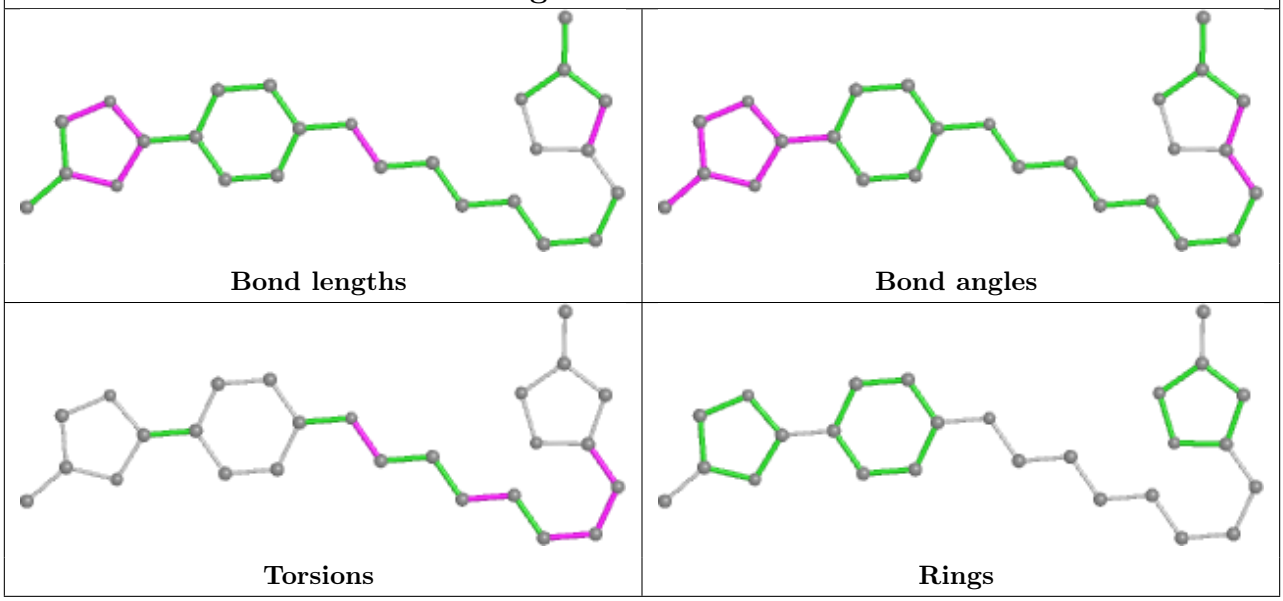
There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	290	W84	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand W84 1 290



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	150:ALA	C	151:MET	N	1.66
1	1	219:SER	C	220:HIS	N	0.90
1	1	220:HIS	C	221:MET	N	0.76

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.